PROGRAM

Second International Alloy Conference (IAC-2)

An Interdisciplinary Approach to the Science of Alloys in Metals, Minerals and Other Materials Systems

August 8-13, 1999
Davos, Switzerland

Conference Co-Chairs:
A. Gonis, A. Meike, K. Rajan and P.E.A. Turchi
Lawrence Livermore National Laboratory

United Engineering Foundation, Inc.
Three Park Avenue, 27th Floor
New York, NY 10016-5902
T: 1-212-591-7836 - F: 1-212-591-7441
E-mail: engfnd@aol.com **www:** http://www.engfnd.org

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K. Rajan
A. Gonis
P. Turchi
A. Meike

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13. SUPPLEMENTARY NOTES

There will be no proceedings for this conference

14. ABSTRACT

This is a second Triennial Conference on the physical, chemical, and mechanical properties of materials, interpreted to mean simple and complex inorganic solids, i.e., metals, semiconductors, and mineral of technological and environmental significance

15. SUBJECT TERMS

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TMS

Sunday, August 8, 1999

5:00 pm - 7:00 pm	Registration
7:00 pm - 9:00 pm	Dinner
9:00 pm - 10:00 pm	Opening Reception

All meals will be at the Cresta Sun Hotel.
All Technical Sessions will be at the Congress Center.

Monday, August 9, 1999

7:00 am - 8:30 am	Breakfast
8:30 am - 8:45 am	Welcome and Introductions Tony Gonis, Conference Co-Chair Norm Stoloff, UEF Technical Liaison Barbara Hickernell, Conferences Director, UEF

Session IA: *Thermodynamics of Alloys: Ordering*
Chairperson: A. Meike

8:45 am - 9:25 am	E. K. H. Salje **Ordering mechanisms in minerals**
9:25 am - 9:45 am	H. Lang **Ordering kinetics in B_2-FeAl**
9:45 am - 10:05 am	V. Vaks **Kinetic features of non-simplest alloy orderings: DO_3, $L1_2$, and $L1_0$ type orderings**
10:05 am - 10:25 am	M. Spanl **Short-range ordering kinetics and microstructural development during post-deformation annealing**
10:25 am - 10:55 am	Coffee Break

Session IA: *Thermodynamics of Alloys: Ordering*
Chairperson: K. Masuda-Jindo

10:55 am - 11:35 am	F. Schmid **Order and disorder phenomena at surfaces of binary alloys**
11:35 am - 11:55 am	R. V. Chepulskyy **Analytical description of the short-range order in alloys with many-body atomic interactions**
11:55 am - 12:15 pm	B. Wuensch **Changes in the atomic coordinates and state of anion and cation order induced by alloying in $Y_2[M(2)_YM(1)_{1-Y}]_2O_7$ solid solution systems**
12:15 pm - 12:35 pm	S. I. Simak **Ordering in Cu_2/NiZn: a first-principles Monte-Carlo study**

Monday, August 9, 1999 (continued)

12:45 pm - 2:00 pm	Lunch
2:00 pm - 4:45 pm	*Ad hoc* sessions and/or free time
4:45 pm	Coffee Service

Session IB: *Thermodynamics of Alloys: Kinetics and diffusion*
Chairperson: G. Grimvall

5:00 pm - 5:40 pm	W. E. Glassley **Using arrested solid-solid multiphase reactions in geological materials to deduce the rate of crystal uplift**
5:40 pm - 6:00 pm	M. Athenes **Kinetics of phase separation in a binary alloy: influence of the atomic mobilities**
6:00 pm - 6:20 pm	K. Rajan **Self Assembly in epitaxial semiconductor alloys**
6:20 pm - 6:40 pm	P. A. Khorzhavyi ***Ab initio* study of vacancies in metals and compounds**
6:40 pm - 7:00 pm	W. Pfeiler **Point defect energies in $L1_2$-ordered Ni_3Al**
7:00 pm - 7:15 pm	Discussion
7:30 pm - 9:00 pm	Dinner
9:00 pm - 10:00 pm	Social Hour

Tuesday, August 10, 1999

7:00 am - 8:00 am	Breakfast

Session IC: ***Thermodynamics of Alloys : phase stability and transformation***

Chairperson: W. E. Glassley

8:00 am - 8:40 am	S. Saxena **Application of synchrotron light, CCD-devices and lasers to the study of materials**
8:40 am - 9:00 am	K. Masuda-Jindo **Effects of continuous atomic displacement on the phase stability of metallic alloys**
9:00 am - 9:20 am	G. Grimvall **Dynamical lattice instabilities in alloy phase diagrams**
9:20 am - 9:40 am	S. Fries **Computational thermodynamics: modelling and applications**
9:40 am - 10:00 am	T. Mohri **Susceptibility near the transition temperature calculated from first-principles**
10:00 am - 10:30 am	**Coffee Break**

Chairperson: D. Papaconstantopoulos

10:30 am - 11:10 am	W. Schweika **Diffuse scattering of Cu-Au alloys: displacements and Fermi-surface effects**
11:10 am - 11:30 am	V. Vinograd **Maximization of cluster entropy via an irreversible algorithm: application to the cluster variation method**
11:30 am - 11:50 am	C. Colinet **CVM calculations of the solid-state equilibria in the Fe-Co phase diagram**
11:50 am - 12:10 pm	S. Shallcross **Onsager cavity field in statistical mechanics of alloys**

Tuesday, August 10, 1999 (continued)

12:30 pm - 2:00 pm	Lunch
2:00 pm - 5:15 pm	*Ad hoc* sessions and/or free time
5:15 pm	Coffee Service

Session II: *Focused Session on Surfaces and Multilayers*

Chairperson: J. S. Faulkner

5:30 pm - 5:50 pm	A. V. Ruban **Random surface alloys: CPA versus super-cell approach**
5:50 pm - 6:30 pm	S. Mahajan **Two-dimensional phase separation and atomic ordering in mixed III-V layers**
6:30 pm - 6:50 pm	Z. Chen **The evaluation of the fracture strain of ITO films on polymeric substrates**
6:50 pm - 7:30 pm	Discussion
7:45 pm - 9:15 pm	Dinner
9:15 pm - 10:15 pm	Social Hour

Wednesday, August 11, 1999

07:00 am - 09:00 am	Breakfast

Session II: ***Focused Session on Surfaces and Multilayers***

Chairperson: T. Mohri

8:00 am - 8:40 am	J. Kudrnovsky ***Ab initio*** **theory of perpendicular transport in magnetic multilayers**
8:40 am - 9:20 am	J. Rustad **Molecular dynamics simulation of iron oxide-water interfaces with classical potentials**
9:20 am - 9:50 am	Coffee Break

Session IC: ***Thermodynamics of Alloys : phase stability and transformation***

Chairperson: K. Rajan

9:50 am - 10:30 am	J. Wong **In-situ chemical dynamics and phase transformation under steep thermal gradients using time-resolved and spatially resolved diffraction**
10:30 am - 10:50 am	B. Bokhonov **Application of transmission electron microscopy for in situ studies of the formation of intermetallic compounds**
10:50 am - 11:10 am	A. V. Ruban **Crystal-structure effect in transition metals and alloys**
11:10 am - 11:30 am	M. Gubinsky **One-stage Copper alloy recuperation from bimetallic pipe waste**
12:00 noon - 7:30 pm	Boxed Lunch and Optional Excursion

Wednesday, August 11, 1999 (continued)

19:00 - 20:30	Dinner
20:30 - 21:30	Social Hour

Thursday, August 12, 1999

7:00 am - 8:00 am	Breakfast

Session III: *Electronic Structure and Properties*
Chairperson: W. H. Butler

8:00 am - 8:40 am	J. S. Faulkner **Tests of the polymorphous coherent potential approximation**
8:40 am - 9:20 am	A. Lodder **Electromigration and electronic structure**
9:20 am - 9:40 am	T. C. Schulthess **Electronic structure and antiferromagnetic ordering in FCC FeMn**
9:40 am - 10:00 am	V. Milman ***Ab initio* study of Aluminosilicate garnets: structure, compressibility, and site disorder**
10:00 am - 10:30 am	**Coffee Break**

Session III: *Electronic Structure and Properties*
Chairperson: S. G. Fries

10:30 am - 11:10 am	D. Papaconstantopoulos **Tight-binding method for metals insulators and semiconductors**
11:10 pm - 11:30 pm	B. Klein **A real-space, finite element approach to large scale electronic structure calculations**
11:30 pm - 11:50 pm	S. Znam **Bond-order potentials for transition metal based binary alloys:titanium-aluminum alloys**
11:50 pm - 12:10 pm	M. Menon **Tight-binding molecular-dynamics studies of relaxation around copper substitutional additive in Ni**
12:10 pm - 12:30 pm	P. James ***Ab initio* calculations of 3d alloys**
12:45 pm - 2:00 pm	Lunch

Thursday, August 12, 1999 (continued)

2:00 pm - 4:45 pm	*Ad hoc* sessions and/or free time
4:45 pm	Coffee Service

Session IV: *Mechanical Properties*
Chairperson: P. E. A. Turchi

5:00 pm - 5:40 pm	A. Lozovoi **Point defects in Al-rich NiAl alloys under pressure**
5:40 pm - 6:00 pm	H. Kokawa **Grain boundary structure dependence of carbide precipitation in sensitized austentic stainless steel**
6:00 pm - 6:20 pm	T. Watanabe **Grain boundary engineering for the control of structure-dependent intergranular oxidation and fracture in nickel-40at% iron alloy**
6:20 pm - 6:40 pm	S. Hanada **Deformation and fracture of TiC/Mo(Nb) in-situ composites**
6:40 pm - 7:00 pm	A. Ohta **Doubled fatigued strength of box welds using low transformation temperature welding material**
7:45 pm - 9:45 pm	Conference Banquet
9:45 pm - 11:00 pm	Social Hour

Friday, June 25, 1999

7:00 am - 9:00 am — Breakfast

Session II: *Focused Session on Surfaces and Multilayers*
Chairperson: A. Gonis

8:00 am - 8:40 am — W. H. Butler
Electronic transport in disordered magnetic multilayers

8:40 am - 9:20 am — B. L. Györffy
Oscillatory magnetic coupling across alloy spacers in metallic multilayers and the corresponding Fermi surface

9:20 am - 10:00 am — J. Tobin
Elementally specific magnetometry of alloys: surfaces and ultra thin films

10:00 am -10:15 am — Gonis, Meike, Rajan, Turchi
Conference Close

12:00 noon — Lunch (or boxed lunch by prior sign-up)

Poster: Surfaces and Multilayers

M. Yandouzi
Thin films NiAl evaporated onto Ag/NaCl study by CTEM and HRTEM

Second International Alloy Conference (IAC-2)
Oral Presentation

DYNAMICAL LATTICE INSTABILITIES IN ALLOY PHASE DIAGRAMS

Goran Grimvall, Theoretical Physics
The Royal Institute of Technology, Stockholm, SE-100 44, Sweden
T: +46-8-7907174, F: +46-8-104879, grimvall@theophys.kth.se

Ab initio electron structure calculations have been widely used to calculate the ground state energy of elements and compounds in various simple lattice structures, and thus account for the observed equilibrium structure. In the early 1990's it was noted that several of the metastable structures of the elements were in fact dynamically unstable under shear. For instance, W has the bcc structure, while fcc W has $c' < 0$. Similarly, Os has the fcc structure but a dynamically unstable bcc lattice with $c' < 0$. Here c' = is Zener's elastic shear constant. With further progress in ab initio calculations, the phonon frequencies $w(q,s)$ could be accurately obtained in the entire Brillouin zone. Dynamical instabilities, i.e. $w^2 < 0$, were frequently found in many lattice structures of high symmetry. This paper discusses our present knowledge about dynamical lattice instabilities in elements, alloys and simple compounds. W-Re alloys are chosen as an illustrating example of the implications for the equilibrium composition-temperature phase diagram.

Second International Alloy Conference (IAC-2)
Oral Presentation

COMPUTATIONAL THERMODYNAMICS: MODELLING AND APPLICATIONS

Suzana G. Fries, ACCESS e.V., RWTH-Aachen
Intzestr. 5, Aachen, D-52072, Germany
T: +49 241 806724, F: +49 241 38578, sufries@aldix.mpi-stuttgart.mpg.de
Bo Sundman, Department of Materials Science and Engineering, Royal Institute of Technology, SE-10044 Stockholm, Sweden
W. Alan Oates, Science Research Institute, University of Salford, Salford M5 4WT, U.K

Thermodynamic databases constructed using the CALPHAD method consist in sets of empirically modelled Gibbs energy functions describing the phases existing in a given multicomponent system.

One advantage of these Gibbsian databases is to be able to calculated phase diagrams (and other thermodynamic properties) which reproduce experimental evidences found in commercial alloys with the precision required by technological applications.

The state of the art of First Principles calculated phase diagram, the theoretical alternative for treating phase stability, is still faraway of such a precision, leaving computational thermodynamics a successful and unique approach for these applications.

An overview will be given about the existing databases, models used, their link to materials, their use in simulations and the improvements that can be acchieved if applications, pragmatic and theoretical approaches can unite.

Second International Alloy Conference (IAC-2)
Oral Presentation

SUSCEPTIBILITY NEAR THE TRANSITION TEMPERATURE CALCULATED FROM FIRST-PRINCIPLES

Tetsuo Mohri, Division of Materials Science and Engineering, Hokkaido University
Kita-13 Nishi-8, Kita-ku, Sapporo, 060-8628, Japan
T: +81-11-706-6348, F: +81-11-706-7812, tmohri@eng.hokudai.ac.jp

There are several experimental evidences of slowing down behavior near the transition temperature for the first-order transition. In order to distinguish it from the conventional critical slowing down phenomenon, they call this as pseudo-critical slowing down phenomenon. The present work is undertaken to reveal the thermodynamic origin of this phenomenon. We employed Path Probability Method and obtained the temperature dependency of the relaxation time for L10-disorder transition. Then, further studied was attempted to calculate the generalized susceptibility near the transition temperature for Cu-Au system by combining Cluster Variation Method with electronic structure calculations. The results indicate that the susceptibility abruptly increases as approaching the transition temperature.

MAXIMIZATION OF CLUSTER ENTROPY VIA AN IRREVERSIBLE ALGORITHM: APPLICATION TO THE CLUSTER VARIATION METHOD. Victor L. Vinograd, Udo Becker, and Andrew Putnis, Institute of Mineralogy, University of Münster, Münster, Germany.

The main difficulty in the cluster variation method is the search for the global free energy minimum in a multi-dimensional space of cluster variables (correlation functions). In models which consider nearest-neighbor (*nn*) interactions only (those within pair, triangle or tetrahedron) the problem can be reduced to two separate tasks:
1) entropy maximization constrained by fixed *nn* correlation functions,
2) free energy minimization with respect to the *nn* correlation functions.

Our presentation shows that the first task can be further reduced to entropy maximization of a basic cluster, while the cluster entropy can be maximized via a set of irreversible operations on cluster probabilities. With the help of the irreversible algorithm the maximum cluster entropy can be found directly as a function of *nn* correlation functions, avoiding explicit introduction of correlation functions of higher-order.

The method allows easy evaluation of high-order CVM approximations for lattices of various topology. The accuracy of the method is discussed in relation to the two-dimensional (square lattice) Ising model.

Contact Author:

Name	Vinograd Victor L.		
Institution	Institute of Mineralogy, Münster University		
Street address	Corrensstrasse 24		
City	Münster	**State/Zip**	48149
Country	Germany	**Tel:**	49-251-8336106 **Fax:** 49-251-8338397
e-mail	vinogra@uni-muenster.de		

Second International Alloy Conference (IAC-2)
Oral Presentation

CVM CALCULATION OF THE SOLID STATE EQUILIBRIA IN THE FE-CO PHASE DIAGRAM

C. Colinet, LTPCM / ENSEEG / INPG
Domaine Universitaire. BP 75, Saint-Martin d'Heres, 38402, France
T: 04 76 82 65 14, F: 04 76 82 67 67, ccolinet@ltpcm.inpg.fr
A. Antoni-Zdziobek, LTPCM / ENSEEG /INPG

Solid state phase equilibria in Fe-Co system are investigated using the CVM method in the irregular tetrahedron approximation in the bcc lattice and in the regular tetrahedron approximation in the fcc lattice. Calculations are performed in the quaternary Fe+Fe-Co+Co- by considering both chemical and magnetic interactions. The A2/B2 order/disorder transition and the alpha/gamma transition agree well with the experimental data in the literature. The composition dependence of the Curie temperatures for bcc and fcc alloys as predicted here are also presented.

Tuesday, August 10, 1999 (continued)

Session II: *Focused Session on Surfaces and Multilayers*
Chairperson: J. S. Faulkner

A. V. Ruban
Random surface alloys: CPA versus super-cell approach

S. Mahajan
Two-dimensional phase separation and atomic ordering in mixed III-V layers

Z. Chen
The evaluation of the fracture strain of ITO films on polymeric substrates

Second International Alloy Conference (IAC-2)
Oral Presentation

CRYSTAL-STRUCTURE EFFECT IN TRANSITION METALS AND ALLOYS

A. V. Ruban, CAMP, Physics Department
Danish Technical University, Lyngby, 2800, Denmark
T: (45) 45 25 32 34, F: (45) 45 93 23 99, ruban@fysik.dtu.dk
H. L. Skriver, Danish Technical University

It is demonstrated that the crystal structure strongly influences thermodynamic properties such as solution, mixing and segregation energies in transition metal alloys. The origin of the strong structural effects is the local character of interatomic bonding which can be accounted for in the virtual-bond model. This model is discussed in application to the solution, mixing and segregation energies.

PHASE SEPARATION AND ATOMIC ORDERING IN MIXED III-V LAYERS

S. Mahajan

Department of Chemical, Bio and Materials Engineering and
Arizona State University
Tempe, AZ 85287-6006

ABSTRACT

It will be shown that atomic species in mixed III-V layers are not distributed at random on their respective sub-lattices. Two types of deviations from randomness are observed: phase separation and atomic ordering. Phase separation occurs on the surface while the layer is growing and is two-dimensional in nature. It cannot be suppressed using non-equilibrium growth techniques, is only observed in layers whose constituents differ in their tetrahedral radii, and its occurrence is governed by surface thermodynamics.

Atomic ordering coexists with phase separation in layers grown by vapor phase techniques. Depending on the prevailing surface reconstruction, double and triple period superlattices develop on {111} planes. It will be argued that the occurrence of surface reconstruction produces sub-surface stresses that bias the occupation of certain sites by atomic species differing in their tetrahedral radii, resulting in atomic ordering. Furthermore, the influence of phase separation and atomic ordering on electronic properties will be discussed.

Second International Alloy Conference (IAC-2)
Oral Presentation

THE EVALUATION OF THE FRACTURE STRAIN OF ITO FILMS ON POLYMERIC SUBSTRATES

Z. Chen, Institute of Materials Research and Engineering
10 Kent Ridge Crescent, Singapore, Singapore, 119260, Singapore
T: +65 874 8193, F: +65 872 0785, z-chen@imre.org.sg
W. Wang, Institute of Materials Research and Engineering
B. Cotterell, Institute of Materials Research and Engineering

One of the mechanical issues concerning flexible organic light emitting device (OLED) is the flexibility, which is controlled by the fracture strength of the brittle films in the device. For example, the integrity of the anode material, the ITO film in the device directly controls the functioning of the device. Understanding the behaviour of these films under flexed condition will help maximize the flexibility of the device. Experiments have been devised to achieve this goal by bending the films of interests to gradually increased curvature over the point of film cracking, both under tension and compression. In this work concentration is given to ITO film. Fracture mechanisms under tension is found to be parallel channelling crack. Under compression the film fails by channelled buckling delamination prior to film cracking, which superficially looks very similar to the tensile cracking if observed under optical microscope or lower-resolution SEM. Based on the understanding of the thin film mechanics on the above phenomena, ways to improve the flexibility are proposed from device design point of view.

Wednesday, August 11, 1999

Session II: *Focused Session on Surfaces and Multilayers*
Chairperson: T. Mohri

J. Kudrnovsky
***Ab initio* theory of perpendicular transport in magnetic multilayers**

J. Rustad
Molecular dynamics simulation of iron oxide-water interfaces with classical potentials

Session IC: *Thermodynamics of Alloys : phase stability and transformation*
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J. Wong
In-situ chemical dynamics and phase transformation under steep thermal gradients using time-resolved and spatially resolved diffraction

B. Bokhonov
Application of transmission electron microscopy for in situ studies of the formation of intermetallic compounds

A. V. Ruban
Crystal-structure effect in transition metals and alloys

M. Gubinsky
One-stage Copper alloy recuperation from bimetallic pipe waste

ABSTRACT FOR IAC-2
August 8-13, 1999 - Davos,Switzerland

Submitted to main topic area: 1

Subtopic area: b. Conductivity/Transport

AB INITIO THEORY OF PERPENDICULAR TRANSPORT IN MAGNETIC MULTILAYERS, **Josef Kudrnovský and Václav Drchal, Institute of Physics ASCR, Prague; Ilja Turek, Institute of Physics of Materials ASCR, Brno; Claudia Blaas and Peter Weinberger, Center for Materials Science, Vienna and Patrick Bruno, Max-Planck Institute for Microstructure Physics, Halle**

The perpendicular magnetoconductance of a trilayer consisting from the sample sandwiched between two ideal leads is developed on *ab initio* level. The sample consists of two magnetic slabs separated by non-magnetic spacer metal. We employ the transmission matrix formulation of the conductance in the framework of the spin-polarized surface Green function technique which fully exploits layered nature of the problem. The electronic structure part of the problem is treated in the framework of the tight-binding linear muffin-tin orbital method generalized to layered systems. The formalism is extended to the case of lateral supercells with random arrangements of atoms in each sample layer which allows to treat both the ballistic and diffusive transport regimes on equal footing. An efficient method for evaluation of the supercell lead surface Green function is presented.

The formalism is applied to fcc-Co/Cu/Co(001) based trilayers with possible disorder of the substitutional type in the spacer, magnetic slabs, and at sample interfaces.

Contact & presenting author:
Full name: Josef Kudrnovský
Institution: Institute of Physics ASCR
Department: Theoretical
Street / PO Box: Na Slovance 2
Zip / City: CZ-182 12 Prague
Country: Czech Republic
Contact address:
J. Kudrnovský
Institute of Physics AS CR
Na Slovance 2
CZ-182 21 Prague, Czech Republic
Phone: +420-2-6605 2905
Fax: +420-2-8588605
E-mail: kudrnov@fzu.cz

☐ Invited talk

Second International Alloy Conference (IAC-2)
Oral Presentation

IN-SITU CHEMICAL DYNAMICS AND PHASE TRANSFORMATION UNDER STEEP THERMAL GRADIENTS USING TIME-RESOLVED AND SPATIALLY RESOLVED DIFFRACTION

Joe Wong, Lawrence Livermore National Laboratory, University of California
PO Box 808, L-356, Livermore, CA, 94551, USA
T: 925 423-6385, F: 925 424-4737, wong10@LLNL.gov

Intense synchrotron x-radiation emitted from stroage rings provides a number of novel experimental probes to study materials structure, synthesis and processing in both time and spatial regimes not readily possible with conventional x-ray sources. This paper describes a couple of such novel tools developed at LLNL for investigating the chemical dynamics and phase transformation during synthesis and materials processing in real time and in-situ with sub-millimeter spatial resolution. These are time resolved x-ray diffraction (TRXRD) and spatially resolved x-ray diffraction (SRXRD). Examples of high tempeerature solid combustion synthesis and phase mapping in the heat affected zone (HAZ) of fusion welds will be discussed in some detail. Future prospects for such in-situ material dynamics research with high brightness 3rd generation synchrotron sources will be outlined.

Second International Alloy Conference (IAC-2)
Oral Presentation

APPLICATION OF TRANSMISSION ELECTRON MICROSCOPY FOR IN SITU STUDIES OF THE FORMATION OF INTERMETALLIC COMPOUNDS.

Bokhonov Boris, Institute of solid state chemistry
Kutateladze 18, Novosibirsk, 630128, Russia
T: 7-383-2-325645, F: 7-383-2-322847, bokhonov@solid.nsk.su
Korchagin Michail, Institute of solid state chemistry

In the present work, transmission electron microscopy was applied to the studies of structural and morphological characteristics during in situ interaction in metal systems. For this purpose, the pairs of interacting substances were chosen so that only one eutectic point was present in their phase diagrams Au-Si(Ge). Besides, the studies in the systems with unlimited solubility (Au-Ni, Cu-Au) and in the systems involving the formation of intermetallic compounds (Ni-Al, Au-Al, Ag-Al, Ni-Si, Ni-Ge) were also performed. Electron microscopic studies were carried out using the samples in which one of the interacting components was single crystal (or polycrystal) film or foil while the second component was present as a crystal particle of small size. The interaction between them was initiated with the help of a special heating unit or by the electron beam in the microscope with increased intensity. The application of this electron microscopic technique allowed us to obtain the data on the aggregate state of the reacting substances, the nature of transported particles and the ways of their transport; to reveal phase composition of the intermediate products and the sequence of stages through which the formation of the final product proceeds. Besides, the observations of the interaction allowed to make conclusions concerning the formation and the development of the defect structure at the interphase boundary between the interacting substances.

Second International Alloy Conference (IAC-2)
Poster Presentation

ONE-STAGE COPPER ALLOY RECUPERATION FROM BIMETALLIC PIPE WASTE

Michailo Gubinskyy, State Metallurgical Academy of Ukraine
11 Pysarzhevsky Str., Apt.71, Dniepropetrovsk, n/a, 320005, Ukraine
T: 380-562-462079, F: 380-562-7702777, tatyana@vved.dp.ua

The major disadvantages of the existing methods of copper alloys recuperation could be confined to the following factors: they result in a pronounced deterioration of a finished product quality, sufficient energy expenditure, multiple stages of production and irretrievable losses of such expensive alloying element as tin. Taking these shortcomings as a point of departure the authors assumed it vital to develop a highly efficient and simple technology of pyrometallurgical recycling of copper based alloys from bimetallic pipe waste.

The steel-copper and steel-bronze pipe production technology analysis shows that 1500 tons of copper-clad bimetallic pipe waste could be recuperated into 150 tons of recycled copper and alloys with the same amount of alloying components as that of virgin materials.

The technology is based on the melting temperature difference between steel and copper-based alloys. Different technological variants have been worked out for the technological temperature range between 1080-1130 C. Serial experiments allowed to define optimal values for the main technological parameters of the process: temperature and speed of heating, velocity of melt excision.

On the basis of experimental investigation the authors designed and tested a pilot unit for continuous non-ferrous metal recycling. The unit operation helped to specify technological regimes and to get representative batches of recycled bronze the content of which was identical to that of a virgin material.

Thursday, August 12, 1999

Session III: *Electronic Structure and Properties*
Chairperson: W. H. Butler

J. S. Faulkner
Tests of the polymorphous coherent potential approximation

A. Lodder
Electromigration and electronic structure

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Electronic structure and antiferromagnetic ordering in FCC FeMn

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***Ab initio* study of Aluminosilicate garnets: structure, compressibility, and site disorder**

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D. Papaconstantopoulos
Tight-binding method for metals insulators and semiconductors

B. Klein
A real-space, finite element approach to large scale electronic structure calculations

S. Znam
Bond-order potentials for transition metal based binary alloys: titanium-aluminum alloys

M. Menon
Tight-binding molecular-dynamics studies of relaxation around copper substitutional additive in Ni

P. James
***Ab initio* calculations of 3d alloys**

Alloy Conference
Submitted to main topic area: 1. Electronic structure and properties
Subtopic area: b. Conductivity/transport

ELECTROMIGRATION AND ELECTRONIC STRUCTURE

A. Lodder,
Department FEW/Natuurkunde en Sterrenkunde
De Boelelaan 1081
1081 HV Amsterdam, The Netherlands

and J.P. Dekker,
Max-Planck Institute für Metallforschung, Stuttgart, Germany

Regarding the two different contributions to the driving force, the direct force and the wind force, the rôle of the electronic structure has been quite different for the two. For the wind force increasingly sophisticated descriptions have been used, namely pseudopotential models, finite cluster models and, at the end, an ab initio Korringa-Kohn-Rostoker Green's function description. We will illustrate this by showing for which systems by now the wind force has been calculated, which include almost all FCC and BCC metals, while both self-electromigration and impurity migration have been treated. Some new results will be presented as well, which simulate electromigration along a grain boundary and over a surface. The direct force, on the other hand, has mainly been discussed in terms of the simple free electron, or jellium model. However, it will be shown that we have arrived at a point, at which more sophisticated descriptions of the electronic structure involved are becoming important. A recent analysis of new experimental results leads to the conclusion, that a migrating hydrogen atom effectively can have a direct valence smaller than unity, depending on the metal studied. By this it becomes challenging to perform calculations of the electronic structure of an interstitial, not only at its equilibrium position, but also at positions lying along the jump path. The barriers for doing so have been abolished recently, since a formulation has been found by which the free electron poles of the interstitial Green's function have become handable.

Second International Alloy Conference (IAC-2)
Oral Presentation

ELECTRONIC STRUCTURE AND ANTIFERROMAGNETIC ORDERING IN FCC FEMN

T. C. Schulthess, Oak Ridge National Laboratory
P.O.Box 2008, Oak Ridge, TN, 37830-6114, USA
T: (423) 574 4344, F: (423) 574 7659, schulthesstc@ornl.gov
W. H. Butler, Oak Ridge National Laboratory
G. M. Stocks, Oak Ridge National Laboratory
S. Maat, University of Alabama
G. J. Mankey, University of Alabama

FCC FeMn is a chemically disordered but antiferromagnetically ordered alloy with face centered cubic structure. These seemingly contradicting facts can be understood in the light of non-collinear magnetic ordering and a first principles treatment of the electronic structure. We use the layer-KKR multiple scattering approach in conjunction with the single site CPA which we have generalized to allow for non-collinear alignment of the moments. We find that three magnetic states could be converged: The collinear 1Q state with alternating (100) planes that are compensated and the non-collinear 2Q and 3Q states, with four ferromagnetic sub-lattices that have their moments pointing along, respectively, the diagonals of the (100) face or along the diagonals of the cube. Both non-collinear states are stable with the 3Q state having the lowest energy. The collinear 1Q state is unstable. The partial densities of states of Fe and Mn are very similar in the non-collinear states with a pseudo gap forming at the Fermi level which in turn stabilizes antiferomagnetic ordering. Research sponsored by the Office of Basic Energy Sciences of the USDOE under contract DE-AC05-96OR22464 with Lockheed Martin Energy Research Corporation. SM and GJM are sponsored by NSF-DMR-94400399 and DOD nano structures DAAH-94-96-1-0316.

Second International Alloy Conference (IAC-2)
Oral Presentation

AB INITIO STUDY OF ALUMINOSILICATE GARNETS: STRUCTURE, COMPRESSIBILITY, AND SITE DISORDER

Victor Milman, MSI
The Quorum, Barnwell Rd, Cambridge, CB5 8RE, UK
T: +44 1223 413300, F: +44 1223 413301, vmilman@msi.com
Bjoern Winkler, Kristallographie / Institut für Geowissenschaften, Olshausenstr 40, D 24098 Kiel, Germany
Chris Pickard, Kristallographie / Institut für Geowissenschaften, Olshausenstr 40, D 24098 Kiel, Germany
Ross Nobes, FECIT, 2 Longwalk Road, Stockley Park, Uxbridge UB11 1AB, UK
Lena Akhmatskaya, FECIT, 2 Longwalk Road, Stockley Park, Uxbridge UB11 1AB, UK

The structural and electronic properties of end-members of the aluminosilicate garnet family (pyrope, grossular, spessartine and almandine) have been investigated as a function of applied pressure. The study has been performed with the density-functional theory code CASTEP which uses pseudopotentials and plane-wave basis set.

The geometrical parameters of the unit cells containing 80 atoms have been fully optimized. The calculated static geometry, bulk modulus and its pressure derivative are in good agreement with the available experimental data. It is shown that the bending of the Si-O-Al angle between the octahedra and tetrahedra is the main compression mechanism for all garnets studied. The non-monotonic dependence of bulk modulus on unit cell volume is explained in terms of differences in compression mechanism for AlO_6 octahedra.

Further, the bonding and dynamics of Mg in pyrope is investigated. The potential at Mg site is strongly anisotropic, and also anharmonic in one direction. The calculations confirm that there is no static 'subsite' disorder of the Mg in pyrope.

The effect of a hydrogarnet substitution, SiO_4 $(OH)_4$, on structure and properties of pyrope and grossular is investigated.

Second International Alloy Conference (IAC-2)
Oral Presentation

DR

Dimitrios Papaconstantopoulos, Naval Research Laboratory
Code 6390, 4555 Overlook Ave. S.W., Washington, DC, 20375, USA
T: 202-767-6886, F: 202-404-7546, papacon@dave.nrl.navy.mil

TIGHT-BINDING METHOD FOR METALS INSULATORS AND SEMICONDUCTORS D. A. Papaconstantopoulos, Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, USA Tight-binding total energy methods bridge the gap between highly accurate, but slow and memory consuming, first-principles density functional calculations and fast, compact, but less accurate atomistic potential methods. Over the past few years we have developed a highly accurate tight-binding method. The environmentally sensitive tight-binding parameters are determined by fitting to the bands structures and total energies of a small number (10-50) first-principles calculations. The resulting Hamiltonian is used to interpolate between these first-principles calculations, allowing highly accurate determinations of structural energy orderings, elastic constants, phonon frequencies, and surface energies. We have also developed computer programs which can use these parameters to do tight-binding molecular dynamics and to determine the electronic structure of a system. In this talk we show typical results for metals,insulators and semiconductors. This work is supported by the U.S. Office of Naval Research and the Department of Defense Common HPC Software Support Initiative (CHSSI) program. Tight-binding total energy methods bridge the gap between highly accurate, but slow and memory consuming, first-principles density functional calculations and fast, compact, but less accurate atomistic potential methods. Over the past few years we have developed a highly accurate tight-binding method. The environmentally sensitive tight-binding parameters are determined by fitting to the bands structures and total energies of a small number (10-50) first-principles calculations. The resulting Hamiltonian is used to interpolate between these first-principles calculations, allowing highly accurate determinations of structural energy orderings, elastic constants, phonon frequencies, and surface energies. We have also developed computer programs which can use these parameters to do tight-binding molecular dynamics and to determine the electronic structure of a system. In this talk we show typical results for metals,insulators and semiconductors. This work is supported by the U.S. Office of Naval Research and the Department of Defense Common HPC Software Support Initiative (CHSSI) program.

Second International Alloy Conference (IAC-2)
Oral Presentation

A REAL-SPACE, FINITE ELEMENT APPROACH TO LARGE-SCALE ELECTRONIC STRUCTURE CALCULATIONS

Barry M. Klein, Department of Physics, University of California
One Shields Avenue, Davis, CA, 95616, USA
T: 530-752-2072, F: 530-752-6359, bmklein@ucdavis.edu
John E. Pask, Department of Physics, University of California, Davis, CA 95616 USA
C. Y. Fong, Department of Physics, University of California, Davis, CA 95616 USA
Philip A. Sterne, Lawrence Livermore National Laboratory, Livermore, CA 94550 CA,

We present an approach to solid-state electronic-structure calculations based on the finite-element method. In this method, the basis functions are strictly local, piecewise polynomials. Because the basis is composed of polynomials, the method is completely general and its convergence can be controlled systematically. Because the basis functions are strictly local in real space, the method allows for variable resolution in real space; produces sparse, structured matrices, enabling the effective use of iterative solution methods; and is well suited to parallel implementation. The method thus combines the significant advantages of both real-space-grid and basis-oriented approaches and so promises to be particularly well suited for large, accurate ab initio calculations. We develop the theory of our approach, discuss advantages and disadvantages, and report initial results, including electronic band structures and details of the convergence of the method. We also present results of studies of positrons in solids using this method, including the calculation of positron lifetimes and comparisons with experiment.

Second International Alloy Conference (IAC-2)
Oral Presentation

BOND-ORDER POTENTIALS FOR TRANSITION METAL BASED BINARY ALLOYS: TI-AL AND MO-SI ALLOYS

S. Znam, Department of Materials Science and Engineering, University of Pennsylvania
3231 Walnut Street, Philadelphia, Pennsylvania, 19104-6272, U.S.A
T: 215-898-9171, F: 215-573-2128, znam@lrsm.upenn.edu
D. Nguyen-Manh, Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK.
D. G. Pettifor, Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK.
V. Vitek, Department of Materials Science and Engineering, University of Pennsylvania

Bond-order potentials (BOPs) for atomistic modelling of lattice defects in materials with mixed metallic and covalent bonding are derived within a parametrized tight-binding framework. BOP is an order N, fully real space method that does not require use of periodic boundary conditions. The cohesive energy is composed of the bond energy that contains the angular dependence of the atomic interactions, an environment dependent central-force many-body term representing the overlap repulsion arising from the valence sp electrons, and a pair potential term representing short-range repulsions. A condition of charge neutrality at individual atoms is employed as an ersatz for self-consistency. For transition metal based alloys BOPs are constructed in which only the valence d-electrons are retained explicitly on the transition metal sites and the p-electrons on the non-transition metal sites. A common feature of these materials is negative Cauchy pressure that is adequately reproduced owing to inclusion of the environmentally dependent term. The tight-binding parameters, the two-center hopping integrals, entering the bond part have been generated by first-principles LMTO calculations that established their transferability. While for Ti-Al alloys these parameters scale simply with the separation of the corresponding atoms, it is shown that in the case of Mo-Si alloys their environmental dependence must be included. Specific potentials for TiAl with the L10 structure are presented and tested by the following studies that have been made in parallel with ab initio calculations: Comparison of competing structures with the same stoichiometry and investigation of complex transformation paths between different structures.

Second International Alloy Conference (IAC-2)
Oral Presentation

TIGHT-BINDING MOLECULAR-DYNAMICS STUDIES OF RELAXATION AROUND COPPER SUBSTITUTIONAL ADDITIVE IN NICKEL

Madhu Menon, University of Kentucky
Department of Physics, Lexington, Kentucky, 40506, USA
T: (606) 257 8737, F: (606) 323 1029, super250@pop.uky.edu
Antonis Andriotis, Institute of Electronic Structure and Laser (FORTH), Heraklion, Crete, Greece 71110

The tight-binding molecular-dynamics (TBMD) simulation scheme for magnetic materials is generalized to include interactions of complex hetero-atomic systems. The data base for fitting the parameters is obtained from {\it ab initio} results for small clusters using the density functional method and the single, double and triple coupled clusters method. Further data base is obtained from experimental results for the bulk solid. The formalism thus developed is used to study electronic properties and lattice relaxation around a substitutional copper atom in a magnetic nickel host.

Thursday, August 12, 1999 (continued)

Session IV: *Mechanical Properties*
Chairperson: P. E. A. Turchi

A. Lozovoi
Point defects in Al-rich NiAl alloys under pressure

H. Kokawa
Grain boundary structure dependence of carbide precipitation in sensitized austentic stainless steel

T. Watanabe
Grain boundary engineering for the control of structure-dependent intergranular oxidation and fracture in nickel-40at% iron alloy

S. Hanada
Deformation and fracture of TiC/Mo(Nb) in-situ composites

A. Ohta
Doubled fatigued strength of box welds using low transformation temperature welding material

Second International Alloy Conference (IAC-2)
Oral Presentation

POINT DEFECTS IN AL-RICH NIAL ALLOYS UNDER PRESSURE

Alexander Y. Lozovoi, The Queen's University of Belfast
University Road, Belfast, Northern Ireland, BT7 1NN, U.K.
T: + 44-(0)1232-273528, F: + 44-(0)1232-241958, s.lozovoi@qub.ac.uk
Ali Alavi, The Queen's University of Belfast
Pavel A. Korzhavyi, Uppsala University
Michael W. Finnis, The Queen's University of Belfast

We investigate the effect of elevated pressures and finite temperatures on the point defect statistics in Al-rich NiAl alloys, where elimination of structural vacancies at high pressure is expected. In doing so we use density functional theory to compute point-defect energies as a function of pressure, which are in turn used as input to the Wagner-Schottky model. We find that at about 200 kbar a change in the constitutional defect takes place from V_{Ni} to Al_{Ni}. We extend the Wagner-Schottky model by introducing elastic interactions between defects, which leads to the prediction of a qualitatively new phenomenon in the system, namely the appearance of an isostructural phase transition terminated at a critical point. Similar behaviour is expected in some other 3/2 Hume-Rothery electron compounds.

Second International Alloy Conference (IAC-2)
Oral Presentation

GRAIN BOUNDARY STRUCTURE DEPENDENCE OF CARBIDE PRECIPITATION IN SENSITIZED AUSTENITIC STAINLESS STEEL

Hiroyuki Kokawa, Tohoku University
Department of Materials Processing, Graduate School of Engineering, Aoba-yama 02, Sendai, Miyagi, 980-8579, Japan
T: +81-22-217-7351, F: +81-22-217-7351, kokawa@material.tohoku.ac.jp
Takashi Koyanagawa, Tohoku University, Now with Toshiba Corporation
Masayuki Shimada, Tohoku University
Yutaka S. Sato, Tohoku University
Takeshi Kuwana, Tohoku University

Grain boundary carbide precipitation and intergranular corrosion in sensitized austenite stainless steel were examined by transmission electron microscopy(TEM) to clarify the effect of grain boundary structure on precipitation and corrosion. A type 304 steel which had been solutionized at 1350 K was heat-treated at temperatures of 800-1300 K. Oxalic acid etch and Strauss tests showed that the frequency of grain boundaries with M23C6 carbide precipitation and corroded boundaries increased with holding time at sensitizing temperatures. The grain boundary carbide precipitation was observed during heat treatment at 1000 K by TEM. Grain boundaries were characterized on the basis of the Coincidence Site Lattice(CSL) theory using electron diffraction Kikuchi patterns. The observations revealed that the propensity to intergranular precipitation depends strongly on the grain boundary structure. Carbide precipitates tend to be detected at grain boundaries with higher sigma-values or larger deviation angles from low sigma CSL misorientations. The border lines between precipitation and no precipitation can be drawn by a parameter of deviation angle divided by the maximum deviation angle by Brandon's criterion. The parameter of border line decreased with the increase in the holding time at 1000 K. This means that the more ordered boundary needs the longer time for carbide precipitation and corrosion than less ordered or random boundaries.

Second International Alloy Conference (IAC-2)
Oral Presentation

GRAIN BOUNDARY ENGINEERING FOR THE CONTROL OF STRUCTURE-DEPENDENT INTERGRANULAR OXIDATION AND FRACTURE IN NICKEL-40AT% IRON ALLOY

T. Watanabe, Tohoku University
Department of Machine Intelligence and Systems Engineering, Aoba-yama 02, Sendai, 980-8579, Japan
T: 81-22-217-6902, F: 81-22-217-6903, watanabe@mdie.mech.tohoku.ac.jp
S. Yamaura, Tohoku University
Y. Igarashi, Tohoku University
S. Tsurekawa, Tohoku University

The most recent studies of structure-dependent intergranular oxidation and of the grain boundary engineering for the control of oxidation-assisted brittleness in polycrystalline materials are discussed. In order to control oxidation-assisted intergaranular fracture which is often an important source of intergranular brittleness of high temperature materials, the effects of grain boundary type and the grain boundary character distribution(GBCD) and grain boundary connectivity on intergaranular oxidation and related fracture have been studied in nickel-40at% iron alloy. It has been found that intergranular oxidation occurs preferentially at high energy random boundaries, while low-energy special boundaries like low sigma coincidence boundaries, particularly sigma 3,11,19,27,31, are highly immune to intergranular oxidation in coarse-grained specimens of the alloy. The effect of grain boundary type and structure on intergranular oxidation was observed to be more significant at a low-oxygen pressure(26ppm O2) than atmospheric pressure(1 atm O2). The effects of the grain boundary character distribution (GBCD) and the grain boundary connectivity have also been studied in rapidly solidified and subsequently annealed polycrystalline ribbons produced by rapid solidification from the melt of the alloy. The frequency of the low energy special boundaries which are resistant to intergranular oxidation and fracture, was increased from 30% to 60% by annealing after rapid solidification. Particular importance of this investigation is the finding that oxidation-assisted intergranular fracture and brittleness of the polycrystalline material can be controlled by engineering the GBCD and the grain boundary connectivity in connection with the grain size.

Second International Alloy Conference (IAC-2)
Oral Presentation

DEFORMATION AND FRACTURE OF TIC/MO(NB) IN-SITU COMPOSITES

Shuji Hanada, Institute for Materials Research, Tohoku University
Katahira 2-1-1, Aoba-ku, Sendai, Miyagi-ken, 980-8577, Japan
T: 81-22-215-2115, F: 81-22-215-2116, hanada@imr.tohoku.ac.jp
Naoyuki Nomura, Institute for Materials Research, Tohoku University
Kyosuke Yoshimi, Institute for Materials Research, Tohoku University

To develop structural materials at very high temperatures over operating temperatures of conventional Ni base superalloys, refractory metal Mo(Nb)-reinforced TiC in-situ composites have been investigated in this study. The isothermal section at elevated temperature of the Ti-Mo-C system shows that TiC(Mo) can be equilibrated with Mo(Ti) in the wide composition field, and a similar tendency can be found in Ti-Nb-C system. Based on these isothermal sections, in-situ composites with various compositions were synthesized by mixing of Nb, Mo and TiC powders followed by arc-melting, and mechanical properties were investigated in relation to their microstructure. Microstructure of arc-melted Mo-40TiC is composed of primary TiC particles and eutectic lamellae consisting of TiC and Mo. Eutectic lamellar structure disappears by substituting Nb for Mo. High temperature compressive strength of the in-situ composites arc-melted can be increased by increasing Mo content to a stress level higher than monolithic TiC at temperatures between 1200 and 1500C. Solidification microstructure is coarsened by directional solidification after arc-melting, which increases creep strength; under a fixed applied stress, minimum creep rate of the directionally solidified composite at 1500C is almost equal to that of conventional Ni base superalloy single crystals at 1100C. Annealing after arc-melting leads to precipitation of fine bcc Mo(Nb) particles in primary TiC particles, thereby reducing the length of cracks introduced by indentation. Directional solidification increases the spacing of bcc Mo(Nb) phase, which raises the fracture toughness at ambient temperature.

Second International Alloy Conference (IAC-2)
Oral Presentation

DOUBLED FATIGUE STRENGTH OF BOX WELDS BY USING LOW TRANSFORMATION TEMPERATURE WELDING MATERIAL

Akihiko OHTA, National Research Institute for Metals
1-2-1 Sengen, Tsukiba-shi, Ibaraki, 305-0047, Japan
T: +81-298-2244, F: +81-298-2201, ohta-a@nrim.go.jp
Naoyuki Suzuki, National Research Institute for Metals
Yoshio Maeda, National Research Institute for Metals

The low transformation temperature welding material is developed to improve the fatigue strength by introducing compressive residaul stress around weld. The developed welding material which contains 10% chromium and 10% nickel, begins to transform from austenite to martensite at about 180 degree centigrade and finishes it at room temperature. During the transformation, the weld metal expands. This expansion induces the compressive residaul stress around the welded part of 20 mm thick JIS SM490B steel plate. The magnitude of welding residaul stress is estimated to be about -100 MPa for developed joint, while that is about 500 MPa for the conventional one. The stress ratio effect due to the compressive residual stress makes the fatigue strength doubled. The fatigue limit for conventional box welds is 65 MPa, while that for developed one is about 130 MPa.

Keywords: Steel, Fatigue, Improvement, Residual stress, Transformation

Friday, June 25, 1999

Session II: *Focused Session on Surfaces and Multilayers*

Chairperson: A. Gonis

W. H. Butler
Electronic transport in disordered magnetic multilayers

B. L. Györffy
Oscillatory magnetic coupling across alloy spacers in metallic multilayers and the corresponding Fermi surface

J. Tobin
Elementally specific magnetometry of alloys: surfaces and ultra thin films

Poster: Surfaces and Multilayers

M. Yandouzi
Thin films NiAl evaporated onto Ag/NaCl study by CTEM and HRTEM

Second International Alloy Conference (IAC-2)
Oral Presentation

ELECTRONIC TRANSPORT IN DISORDERED MAGNETIC MULTILAYERS

W. H. Butler, Oak Ridge National Laboratory
Building 4500S, Mail Stop 6114, Oak Ridge, TN, 37830, USA
T: 423 574 4845, F: 423 574 7659, bhb@ornl.gov
X.-G. Zhang, Oak Ridge National Laboratory
T. C. Schulthess, Oak Ridge National Laboratory
J. M. MacLaren, Tulane University

Electronic transport in magnetic multilayers has received considerable attention since the dicovery of the giant magnetoresistance (GMR) effect. Recently, there have been observations of very large values of GMR[1] in sputtered single crystalline films. These films are of interest to alloy theorists because they apparently are of sufficient perfection that the major process which limits the electron lifetime at low temperature is impurity or alloy scattering. In order to investigate this regime we have calculated the electrical resistivity and giant magnetoresistance of cobalt-copper (100)

Second International Alloy Conference (IAC-2)
Oral Presentation

PROF

B. L. Gyorffy, H. H. Wills Physics Laboratory, Univ. of Bristol
Royal Fort, Tyndall Avenue, Bristol, BS8 1TL, U.K.
T: +44 117 928 8704, F: +44 117 925 5624, b.gyorffy@bristol.ac.uk
N. N. Lathiotakis, H. H. Wills Physics Laboratory, Univ. of Bristol

A theoretical model, based on the screened KKR formalism, is developed for studying the exchange interaction of two semi-infinite layers separated by a non-magnetic metallic spacer layer which is either pure metal or binary alloy. First applications of the model for pure Cu, as well as Cu-Ni and Cr-V alloy spacers are also presented.

Second International Alloy Conference (IAC-2)
Oral Presentation

ELEMENTALLY SPECIFIC MAGNETOMETRY OF ALLOYS: SURFACES AND ULTRA THIN FILMS

James G. Tobin, Lawrence Livermore National Lab
7000 East Ave, POB 808, L-357, Livermore, CA, 94550, USA
T: 925-422-7247, F: 925-423-7040, Tobin1@LLNL.gov

Nanoscale magnetic systems such as Giant Magneto-Restrictive (GMR) and Spin-Valve Materials are miniature, complex, multilayed structures composed of a variety of alloys and elements. To sort out the atomic scale structure-property relationships in such devices and their simplified analogs, elemental specificity is a necessity. Obviously, magnetic sensitivity is also required. One way to obtain a combination of these characteristics is to perform magnetic dichroism in core level spectroscopy, e.g. x-ray absorption [1,2] or photoelectron spectroscopy [3]. Typically, the chirality that gives rise to ferromagnetic sensitivity is induced via the use of circularly polarized x-rays. However, it is also possible to set up a vectorial chirality in angle resolved experiments such as photoemission, using linearly polarized x-rays. [4-7] Because of the intrinsic limitations [8] of the Sum Rule [9,10] based analyses of absorption data, we have taken a dual track approach based upon a combined analysis using Circular Dichroism in Absorption [11] and Linear Dichroism in Photoemission. [12,13] Particular emphasis will be placed upon the discussion of 3d magnetic binary alloys composed of Ni, Fe and Co and their structure - property relationships. [12] [1]Phys. Rev. Lett. 58, 737 (1987); Phys. Rev. Lett. 62, 2620 (1989). [2]Phys. Rev. B. 42, 7262 (1990). [3]Phys. Rev. Lett. 65, 492 (1990). [4]Phys. Rev. Lett. 70, 3479 (1993); Solid State Commun. 86 647 (1993). [5]Phys. Rev. B 49, 15 682 (1994); Solid State Commun. 90, 557 (1994). [6]Phys. Rev. B51, 609 (1995). [7]J. Appl. Phys. 79, 5626 (1996); J. Vac. Sci. Tech. B14, 3171 (1996). [8]Phys. Rev. B 52, 6530 (1995) ; Phys. Rev. Lett. 68, 3642 (1992). [9]Phys. Rev. Lett. 68, 1943 (1992). [10]Phys. Rev. Lett. 70, 694 (1993). [11]J. Vac. Sci. Tech. A 15, 2287 (1997). [12]Phys. Rev. Lett. 79, 5166 (1997). [13]Phys. Rev. Lett. 81, 1306 (1998).

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Alloy Conference

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PARTICIPANTS LIST

ATHENES, MANUEL
Commissariat a L'Energie
Atomique, DECM/SRMP
91191 Gif-Sur-Yvette Cedex
FRANCE
Tel: 33-1-6908-3769
Fax: 33 -1-6908-6867
E-mail: mathenes@cea.fr

CHEPULSKYY, ROMAN V.
National Academy of Sciences
Solid State Theory Dept.
36, Acad. Vernadsky Blvd.
Kiev 142, 252680, UKRAINE
Tel: 380-44-444-9513
Fax: 380-44-444-2561
E-mail: chep@imp.kiev.ua

FAULKNER, J. S.
Florida Atlantic University
Dept. of Physics
Boca Raton, FL 33431
Tel: 561-297-3429
Fax: 561-297-2662
E-mail: faulkner@fau.edu

GLASSLEY, WILLIAM
Geochemist
Lawrence Livermore Nat'l. Lab
7000 East Avenue
Livermore, CA 94550
Tel: 925-422-6499
Fax: 925-422-4918
E-mail: glassleyl@llnl.gov

CHEN, ZHONG
IMRE
(Inst. of Materials Res & Eng)
Science Drive 4, Lvl 3, Bl S7
Singapore 119260, SINGAPORE
Tel: 65-874-8193
Fax: 65-872-0785
E-mail: z-chen@imre.org.sg

COLINET, CATHERINE
Professor
LTPCM/ENSEFG
Domaine Universitaire BP 75
Saint Martin d'Heres 38402, FRANCE
Tel: 33-4-7682-6514
Fax: 33-4-7682-6767
E-mail: ccolinet@ltpcm.inpg.fr

FRIES, SUZANA G.
Access e.V., RWTH-Aachen
Intzestrasse 5
D-52072 Aachen, GERMANY
Tel: 49-241-806-724
Fax: 49-241-385-78
E-mail: sufries@aldix.mpi-stuttgart.mpg.de

GONIS, ANTONIOS
Lawrence Livermore Nat'l Labs.
L-353
Livermore, CA 94551
Tel: 925-422-7150
Fax: 925-423-7040
E-mail: gonis1@llnl.gov

PARTICIPANTS LIST

GRIMVALL, GORAN
Royal Institute of Technology
Theoretical Physics
SE-10044 Stockholm, SWEDEN
Tel: 46-8-790-7174
Fax: 46-8-10-4879
E-mail: grimvall@theophys.kth.se

GYORFFY, BALAZS L.
H.H. Wills Physics Laboratory
Tyndall Avenue
Bristol BS8 1TL, UNITED KINGDOM
Tel: 44-117-928-8704
Fax: 44-117-925-5624

HANADA, SHUJI
Professor
Tohoku University
Inst. for Materials Science
Katahira 2-1-1 Aoba-ku
Sendai, 980-8577, JAPAN
Tel: 81-22215-2115
Fax: 81-22215-2116
E-mail: hanada@imr.tohoku.jp

HICKERNELL, BARBARA K.
Conferences Director
United Engineering Foundation
3 Park Avenue
27th Floor
New York, NY 10016-5902
Tel: 212-591-7836
Fax: 212-591-7441
E-mail: engfnd@aol.com

JINDO, KINICHI M.
Research Fellow
Tokyo Institute of Technology
Material Science Department
Nagatsuta 4259, Midori-ku
Yokohama 226-8502, JAPAN
Tel: 81-45-924-5636
Fax: 81-424-75-0650
E-mail: wmfjindo@din.or.jp

KLEIN, BARRY
Vice Provost
University of California
One Shields Avenue
Davis, CA 95616
Tel: 530-752-2072
Fax: 530-752-6359
E-mail: bmklein@ucdavis.edu

KOKAWA, HIROYUKI
Professor
Tohoku University
Materials Processing Dept.
Aoba-yama 02
Sendai 980-8579, JAPAN
Tel: 81-22-217-7351
Fax: 81-22-217-7351
E-mail: kokawa@material.tohoku.ac.jp

KORZHAVYI, PASHA A.
Uppsala University
Condensed matter Theory Group.
Physics Dept. P.O. Box 530
Uppsala S-751- 21, SWEDEN
Tel: 46-18471-7304
Fax: 46-18511-784
E-mail: kpa@fysik.uu.se

KUDRNOVSKY, JOSEF
Institute of Physics AS CR
Na Slovance 2
CZ-182 21 Prague 8, CZECH REPUBLIC
Tel: 420-2-6605-2905
Fax: 420-2-821-227
E-mail: kudrnov@fzu.cz

LANG, HUBERT
University of Vienna
Institut fur Materialphysik
Strudlhofgasse 4
A-1090 Vienna, AUSTRIA
Tel: 43-131-367-3209
Fax: 43-1-42-779-513
E-mail: bihu@netway.at

PARTICIPANTS LIST

LODDER, ADRI
Professor
Vrije Universiteit
De Boelelaan 1081
1081 HV Amsterdam, THE NETHERLANDS
Tel: 31-204-447-854
Fax: 31-204-447-992
E-mail: alod@nat.vu.nl

LOZOVOI, ALEXANDER Y.
Queen's University of Belfast
School of Maths & Physics
University Road
Belfast BT7 1NN, UNITED KINGDOM
Tel: 44-1232-273-528
Fax: 44-1232-241-958
E-mail: s.lozovoi@qub.ac.uk

MEIKE, ANNEMARIE
Lawrence Livermore Nat'l Lab
L-201
Livermore, CA 94551
Tel: 925-422-3735
Fax: 925-423-1057
E-mail: meike1@llnl.gov

MILMAN, VICTOR
Project Leader, Quantum Mech.
Molecular Simulations Inc.
The Quorum
Barnwell Road
Cambridge CB5 8RE, UNITED KINGDOM
Tel: 44-1223-413-300
Fax: 44-1223-413-301
E-mail: vmilman@msi.com

OHTA, AKIHIKO
Leader of First Unit
Nat'l. Research Institute
Strength & Life Evaluation
1-2-1 Sengen, Tsukuba-shi
Ibaraki 305-0047, JAPAN
Tel: 81-298-59-2244
Fax: 81-298-59-2201
E-mail: ohta-a@nrim.go.jp

LOPEZ, HUGO F
Associate Professor
University of Wisconsin
Materials Department
P.O. Box 784
Milwaukee, WI 53201
Tel: 414-229-6005
Fax: 414-229-6958
E-mail: hlopez@uwm.edu

MAHAJAN, SUBHASH
Professor
Arizona State University
Dept. of Chemical, Biology and
Materials Engineering
Tempe, AZ 85287-9710
Tel: 480-965-9710
Fax: 480-965-0037
E-mail: smahajan@asu.edu

MENON, MADHU
University of Kentucky
Physics Department
Lexington, KY 40506
Tel: 606-257-8737
Fax: 606-323-1029
E-mail: super250@pop.uky.edu

MOHRI, TETSUO
Professor
Hokkaido University
Graduate School of Engineering
Kita-13, Nishi-8, Kita-ku
Sapporo 060-8628, JAPAN
Tel: 81-11-706-6348
Fax: 81-11-706-7812
E-mail: tmohri@eng.hokudai.ac.jp

PAPACONSTANTOPOULOS, DIMITRIOS
Naval Research Lab.
Center for Computational
Materials Science, Code 6390
Washington, DC 20375
Tel: 202-767-6886
Fax: 202-404-7546
E-mail: papacon@dave.nrl.navy.mil

PARTICIPANTS LIST

PFEILER, WOLFGANG
University of Vienna
Institut fur Materialphysik
Strudlhofgasse 4
A-1090 Vienna, AUSTRIA
Tel: 43-131367-3209
Fax: 43-1-42-779-513
E-mail: pfeiler@ap.univie.ac.at

RUBAN, ANDREI
Tech. University of Denmark
CAMP, Physics Department
Bldg. 307
Lyngby 2800, DENMARK
Tel: 45-4525-3234
Fax: 45-4593-2399
E-mail: ruban@fysik.dtu.dk

SALJE, EKHARD K.
Head of Department
Cambridge University
Earth Sciences Department
Downing Street
Cambridge CB2 3E2, UNITED KINGDOM
Tel: 44-1223-333-481
Fax: 44-1223-333-478
E-mail: es10002@esc.cam.ac.uk

SCHMID, FREIDERIKE
Max-Planck-Institut
Polymerforschung
Ackermannweg 10
D-55021 Mainz, GERMANY
Tel: 49-6131-379-218
Fax: 49-6131-379-340
E-mail: schmid@mpip-mainz.mpg.de

SCHWEIKA, WERNER
Institut fur Streumethoden
IFF, Forschungszentrum Julich
D-52425 Julich, GERMANY
Tel: 49-2461-61-6650
Fax: 49-2461-61-2610
E-mail: w.schweika@fz-juelich.de

RAJAN, KRISHNA
Professor
Rensselaer Polytechnic Inst.
Materials Science & Engrg.
110 8th Street
Troy, NY 12180-3590
Tel: 518-276-6126
Fax: 518-276-8554
E-mail: rajank@rpi.edu

RUSTAD, JAMES
Pacific Northwest Laboratory
MS-K8-96
P.O. Box 999
Richland, WA 99352
Tel: 509-376-3979
Fax: 509-376-3650
E-mail: james.rustad@pnl.gov

SAXENA, SURENDRA
Professor
Uppsala University
Theoretical Geochemistry
Geocentrum, Villavaegen 16
SE-75236 Uppsala, SWEDEN
Tel: 46-18-471-2559
Fax: 46-18-471-2591
E-mail: sksaxena@mail.anst.uu.se

SCHULTHESS, THOMAS C.
Oak Ridge National Laboratory
Metals and Ceramics
MS-6114, 4500 South
Oak Ridge, TN 37831
Tel: 423-574-4244
Fax: 423-574-7659
E-mail: schulthesstc@ornl.gov

SHALLCROSS, SAMUEL
Bristol University
H.H. Wills Physics Laboratory
Tyndal Avenue
Bristol BS8 1T1, UNITED KINGDOM
Tel: 44-117-428-3668
Fax: 44-117-925-5624
E-mail: s.shallcross@bris.ac.uk

PARTICIPANTS LIST

SPANL, MARKUS
University of Vienna
Institut fur Materialphysik
Strudlhofgasse 4
A-1090 Vienna, AUSTRIA
Tel: 43-131-367-3209
Fax: 43-1-42-779-513
E-mail: spanl@ap.univie.ac.at

TOBIN, JAMES G.
Chemist
Lawrence Livermore Nat'l. Lab.
P.O. Box 808, L-357
7000 East Avenue
Livermore, CA 94550
Tel: 925-422-7247
Fax: 925-423-7040
E-mail: tobin1@llnl.gov

TURCHI, P.E.A.
Lawrence Livermore Nat'l Labs.
L-353
Livermore, CA 94551
Tel: 925-422-9925
Fax: 925-423-7040
E-mail: turchi@melun.llnl.gov

VINOGRAD, VICTOR
Institut fuer Mineralogie
Universitat Munster
Corrensstrasse 24, 48149
Munster, GERMANY
Tel: 49-251-8336106
Fax: 49-251-8338397
E-mail: vinogra@uni-muenster.de

WONG, JOE
Lawrence Livermore Nat'l. Lab.
P.O. Box 808
L-356
Livermore, CA 94551
Tel: 925-423-6385
Fax: 925-424-4737
E-mail: wong@cms1.llnl.gov

STOLOFF, NORMAN S.
Professor Emeritus
Rensselaer Polytechnic Inst.
Materials Sci. & Engrg. Dept.
Troy, NY 12180-3590
Tel: 518-276-6436
Fax: 518-276-8554
E-mail: stolon@rpi.edu

TSUREKAWA, SADAHIRO
Associate Professor
Tohoku University
Aramaki-Aza-Aoba 01
Sendai
Miyagi 980-8579, JAPAN
Tel: 81-22-217-6904
Fax: 81-22-217-6904
E-mail: turekawa@mdie.mech.tohoku.ac.jp

VAKS, V.
RRC Kurchatov Institute
Moscow 123182, RUSSIA
Tel: 7-095-1969826
Fax: 7-095-8825804
E-mail: vaks@mbslab.klae.ru

WATANABE, TADAO
Professor
Tohoku University
Machine Intelligence Dept.
Sendai
980-8579 Miyagi, JAPAN
Tel: 81-22-217-6902
Fax: 81-22-217-6903
E-mail: watanabe@mdie.mech.tohoku.ac.jp

WUENSCH, BERNHARDT J.
Professor
M.I.T.
Ceramics Division 13-4037
77 Massachusetts Avenue
Cambridge, MA 02139-4307
Tel: 617-253-6889
Fax: 617-253-5827
E-mail: wuensch@mit.edu

PARTICIPANTS LIST

ZNAM, STEFAN
Graduate Student
University of Pennsylvania
Materials Science & Engrg.
Philadelphia, PA 19104
Tel: 215-898-7883
Fax: 215-573-2128
E-mail: znam@lrsm.upenn.edu

Abstract for IAC-2

Submitted to main topic area: 2. Thermodynamic properties
Subtopic area: 2.b. Ordering and phase transformations

ORDERED STATES AND PHASE TRANSITIONS IN INTERMETALLICS AND THIN METALLIC FILMS, R. Banerjee, S. Amancherla, S.A. Dregia, S. Banerjee*, and H.L. Fraser, Department of Materials Science and Engineering, Ohio State University, 2041 College Road, Columbus, OH 43210, USA. *BARC, Trombay, India

Intermetallic compounds have been the subject of great interest in the past several years as candidate materials in structural applications. Since useful versions of these materials will be alloyed such that their compositions will not represent stoichiometry, it is important to develop means of describing their ordered state. For example, it is important to know and also predict the site occupancies of the various alloying elements. In addition to bulk forms, these materials will find application as thin films or in multilayered configurations. Since it has been demonstrated in several systems that materials can undergo phase transitions as a function of scale, it is important for these types of materials that the occurrence of these possible transitions be determined and predicted. This paper addresses both of these problems and presents simple thermodynamic models which may be used as predictive tools.

Contact Author: Hamish L. Fraser
The Ohio State University
Department of Materials Science and Engineering
2041 College Road
Columbus, OH 43210
USA

Oral session (invited presentation)